Electronic Supplementary Material (ESI) for Analytical Methods.

Table S1 The differentially expressed metabolites in human thyroid cancer cells by ultra-high performance liquid chromatography-mass spectrometry metabolomic profiles.

Ion form	Rt(min)	m/z	Formula	Proposed compound	HMDB	p value	Trend before treatment
$[M+H]^+$	2.78	347.22	$C_{21}H_{30}O_4$	Corticosterone	HMDB01547	8.69E-13	↑
$[M+H]^+$	8.22	256.26	$C_{16}H_{33}NO$	Palmitic amide	HMDB12273	7.74E-13	↓
$[M+H]^+$	9.58	380.26	$C_{18}H_{38}NO_5P$	Sphingosine 1-phosphate	HMDB00277	1.41E-07	↓
$[M+H]^+$	9.87	494.32	$C_{24}H_{48}NO_7P$	LysoPC(16:1(9Z))	HMDB10383	2.30E-05	↑
$[M+H]^+$	10.06	482.32	$C_{23}H_{48}NO_7P$	LysoPC(15:0)	HMDB10381	9.52E-11	↓
$[M+H]^+$	10.21	544.34	$C_{28}H_{50}NO_7P$	LysoPC(20:4(5Z,8Z,11Z,14Z))	HMDB10395	3.69E-10	↓
$[M+H]^+$	10.32	400.34	$C_{23}H_{45}NO_4$	L-Palmitoylcarnitine	HMDB00222	1.11E-16	↓
$[M-H]^-$	1.03	243.06	$C_9H_{12}N_2O_6$	Uridine	HMDB00296	2.76E-14	↑
$[M-H]^-$	4.13	212.00	$C_8H_7NO_4S$	Indoxyl sulfate	HMDB00682	1.71E-06	↓
$[M+H]^+$	9.93	437.29	C24H40O4	3a,12b-Dihydroxy-5b-cholanoic acid	HMDB00364	1.13E-10	↓
$[M+H]^+$	11.68	480.31	$C_{23}H_{48}NO_7P$	LysoPE(18:0/0:0)	HMDB11130	0.000313925	↓
$[M-H]^-$	0.60	125.01	$C_2H_7NO_3S$	Taurine	HMDB00251	0.00015987	↑
$[M-H]^-$	0.63	117.15	$C_5H_{11}NO_2$	L-Valine	HMDB00883	0.001283762	↓
$[M+H]^+$	0.65	114.07	$C_4H_7N_3O$	Creatinine	HMDB00562	2.75E-08	↑
$[M+H]^+$	0.66	158.12	$C_4H_6N_4O_3$	Allantoin	HMDB00462	3.88E-12	↓
$[M-H]^-$	0.73	242.23	$C_{10}H_{14}N_2O_5$	Thymidine	HMDB00273	2.85E-14	↓
$[M-H]^-$	0.90	216.24	$C_8H_{16}N_4O_3$	N-a-acetyl-L-arginine	HMDB04620	6.58E-05	↑
$[M-H]^-$	1.01	146.10	$C_6H_8O_5$	Oxoglutaric acid	HMDB02070	0.026311686	↑
$[M+H]^+$	2.47	165.08	C6H12O5	L-Fucose	HMDB00174	2.54E-12	↑

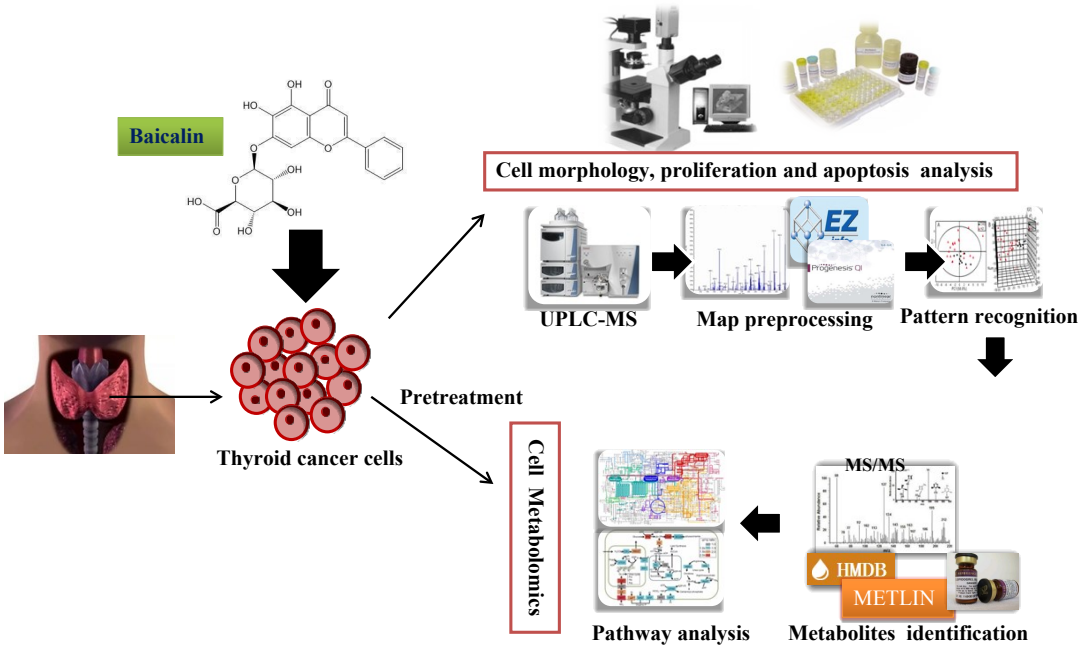

Figure S1 The flow diagram of this study based on high-throughput ultra-high performance liquid chromatography-mass spectrometry cell metabolomic profiles strategy.

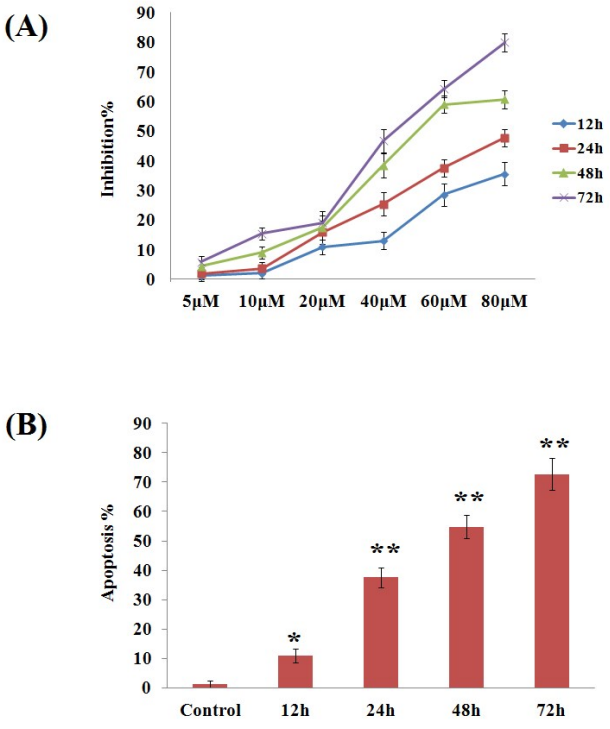

Figure S2 (A) Baicalin caused the cell morphological changes on human thyroid cancer cells as the time change. (B) Baicalin inhibited the proliferation of SW579 human thyroid cancer cells at the concentrations of 5 μM, 10 μM, 20 μM, 40 μM, 60μM, 80μM for 12h,24 h, 48 h, 72 h. (C) Baicalin at the concentrations of 80 μM induce the apoptosis rate change of SW579 human thyroid cancer cells for 12h, 24 h, 48 h, 72 h.